

# [O II] line ratios

Anil K. Pradhan<sup>1</sup>, Maximiliano Montenegro<sup>1,2</sup>, Sultana N. Nahar<sup>1</sup>, Werner Eissner<sup>3</sup>

<sup>1</sup> *Department of Astronomy,* <sup>2</sup> *Department of Education, The Ohio State University, Columbus, OH 43210, USA,*

<sup>3</sup> *Institut für Theoretische Physik, Teilinstitut 1, 70550 Stuttgart, Germany*

Accepted xxxxxx Received xxxxxx; in original form xxxxxx

## ABSTRACT

Based on new calculations we reconfirm the low and high density limits on the forbidden fine structure line ratio [O II]  $I(3729)/I(3726)$ :  $\lim_{N_e \rightarrow 0} = 1.5$  and  $\lim_{N_e \rightarrow \infty} = 0.35$ . Employing [O II] collision strengths calculated using the Breit-Pauli R-matrix method we rule out any significant deviation due to relativistic effects from these canonical values. The present results are in substantial agreement with older calculations by Pradhan (1976) and validate the extensive observational analysis of gaseous nebulae by Copetti and Writzel (2002) and Wang *et al.* (2004) that reach the same conclusions. The present theoretical results and the recent observational analyses differ significantly from the calculations by MacLaughlin and Bell (1998) and Keenan *et al.* (1999). The new maxwellian averaged effective collision strengths are presented for the 10 transitions among the first 5 levels to enable computations of [O II] line ratios.

**Key words:** Gaseous Nebulae – Optical Spectra: H II Regions – Line Ratios: Atomic Processes – Atomic Data

## 1 INTRODUCTION

The most prominent density diagnostics in astrophysics is due to the forbidden fine structure lines [O II]  $\lambda\lambda$  3729, 3726 and [S II]  $\lambda\lambda$  6716, 6731. Their utility stems from several factors such as: (A) they respectively lie at the blue and the red ends of the optical spectrum, (B) their atomic structure and hence the density dependence is essentially the same, and (C) they are quite strong in the spectra of most H II regions owing to the relatively large abundances of oxygen and sulphur. Seaton and Osterbrock (1957) have described the basic physics of these forbidden transitions. High-accuracy calculations using the then newly developed computer programs based on the close-coupling method IMPACT (Eissner and Seaton 1972, 1974, Creeves *et al.* 1978) were later carried out by Pradhan (1976; hereafter P76) for the collision strengths, and by Eissner and Zeippen (1981) and Zeippen (1982) for the transition probabilities. These atomic parameters subsequently enabled a consistent derivation of electron densities from observations of [O II] and [S II] lines in a wide variety of H II regions (e.g. Kingsburgh & English 1992, Aller & Hyung 1995, Aller *et al.* 1996, Keyes *et al.* 1990).

More recently, McLaughlin and Bell (1998; hereafter MB98) repeated the [O II] calculations of collision strengths using the R-matrix method (Burke *et al.* 1971; Berrington *et al.* 1995), also based on the close coupling approximation and widely employed for a large number of atomic calculations (*The Opacity Project Team 1995*, Hummer *et al.* 1993). They included a much larger target wavefunction expansion

than P76, and relativistic effects not considered in the earlier calculations. Their electron impact collision strengths and rate coefficients were markedly different for the relevant transitions  $^4S_{3/2} \rightarrow ^2D_{5/2,3/2}$  than P76, which leads to the theoretical density diagnostic line ratio  $I(3729)/I(3726)$  to be up to 30% higher and  $\approx 2.0$  in the low-density limit  $\lim_{N_e \rightarrow 0}$ . Keenan *et al.* (1999; hereafter K99) recomputed the [O II] line ratios to analyze several planetary nebulae using these MB98 results.

However, other extensive observational studies (e.g. Copetti and Writzel 2002, Wang *et al.* 2004) have noted the discrepancy between electron densities derived from [O II] and other density indicators, notably the [S II]  $\lambda\lambda$  6716, 6731. In particular the recent analysis of a sample of over a hundred nebulae by Wang *et al.* (2004) shows that the collision strengths of MB98 are not supported by observations, and that the earlier results of P76 are to be preferred. But these observational studies leave open the question of what precisely are the collision strengths. Given that P76 used a small basis set to describe the O II target, considered no relativistic effects, and could not fully resolve the resonance structures in the collision strengths owing to computational constraints, it seems puzzling that the new MB98 results which do account for all of these factors appear to be inaccurate.

To address this important issue and to resolve the outstanding discrepancy, we recently undertook new calculations for [O II] using the same Breit-Pauli R-matrix method as employed by MB98 and including relativistic effects. While the

details of the atomic calculations and comparison of collision strengths with different basis sets of target wavefunctions will be presented elsewhere (Montenegro *et al.* 2005), we present the final results of astrophysical interest in this Letter.

## 2 THEORY AND COMPUTATIONS

Forbidden lines are often sensitive to ambient electron density; as the Einstein spontaneous decay rates of the upper levels are small, they may be collisionally excited to other levels by electron impact before radiative decay (Osterbrock 1989, Dopita and Sutherland 2003). This is likely to happen when there is a pair of lines originating from closed spaced metastable energy levels, especially in ions of the  $2p^3$  and the  $3p^3$  outer electronic configurations as exemplified by O II and S II. The first five levels are:  $^4S_{3/2}^o$ ,  $^2D_{5/2,3/2}^o$ ,  $^2P_{3/2,1/2}^o$ . The pair of [O II] transitions of interest are  $^2D_{5/2,3/2}^o \rightarrow ^4S_{3/2}^o$  at  $\lambda 3729$  and  $\lambda 3726$  respectively.

The basic physics of the limiting values of the line ratio  $I(3729)/I(3726)$  is quite simple. At low electron densities every excitation to the two metastable levels  $^2D_{5/2,3/2}^o$  is followed by a spontaneous decay back to the ground level  $^4S_{3/2}^o$  since the collisional mixing rate among the two excited levels is negligible. In that case the line ratio in principle must be equal to the ratio of the excitation rate coefficients

$$\lim_{N_e \rightarrow 0} \frac{I(3729)}{I(3726)} = \frac{q(^4S_{3/2}^o - ^2D_{5/2}^o)}{q(^4S_{3/2}^o - ^2D_{3/2}^o)}, \quad (1)$$

where the excitation rate coefficient  $q_{ij}$  is

$$q_{ij}(T) = \frac{8.63 \times 10^{-6} \text{ cm}^3/\text{s} \cdot \exp(-E_{ij}/kT_e)}{g_i \sqrt{T_e/K}} \Upsilon_{ij}(T_e), \quad (2)$$

where  $g_i$  is the statistical weight of the initial level and the quantity  $\Upsilon_{ij}$  is the Maxwellian averaged collision strength:

$$\Upsilon_{ij}(T) = \int_{E_j}^{\infty} \Omega_{ij}(E) \exp(-E/kT_e) d(E/kT_e). \quad (3)$$

If relativistic effects are negligible then the collision strengths may be calculated in  $LS$  coupling, and an algebraic transformation may be employed to obtain the fine structure collision strengths. This was the procedure employed in P76. The ratio of fine structure  $LSJ$  to  $LS$  collision collision is especially simple when the lower level has either  $L$  or  $S = 0$ , such as for O II and S II, i.e.

$$\frac{\Omega(SLJ - S'L'J')}{\Omega(SL - S'L')} = \frac{2J' + 1}{(2S' + 1)(2L' + 1)}. \quad (4)$$

If the excited levels are so closely spaced that the excitation rates have virtually the same temperature dependence, the line ratio would then be equal to the ratio of the statistical weights  $(2J'+1)$  of the upper levels  $^2D_{5/2,3/2}^o$ , i.e.  $6/4$ . If, however, relativistic mixing is significant then the line ratio will depart from the  $LS$  coupling value. That was the contention of MB98 and K99.

Therefore we carry out the present calculations including relativistic effects and with a suitably large target wavefunction expansion. The Breit-Pauli R-matrix (BPRM) calculations with different trial basis sets are described in detail in another paper (Montenegro

*et al.* 2005). In the present calculations we employ a 16-level target:  $1s^2 2s^2 [2p^3 (^4S_{3/2}^o, ^2D_{5/2,3/2}^o, ^2P_{3/2,1/2}^o); 2s2p^4 (^4P_{5/2,3/2,1/2}, ^2D_{5/2,3/2}), 2p^2 3s (^4P_{1/2,3/2,5/2}, ^2P_{1/2,3/2}), 2s2p^4 (^4S_{1/2})]$ . This close coupling expansion is more than sufficient to obtain accurate collision strengths for the first 5 levels. All resonance structures up to the highest target threshold energy  $E(2s2p^4 (^4S_{1/2})) = 1.7829$  Ry are resolved. The last threshold lies sufficiently high to ensure that resonance and coupling effects in the collision strengths are fully accounted for in the excitation of the first 5 levels considered in the collisional-radiative model to compute the line ratios. Collision strengths at energies 1 Ry higher than the highest of the first 5 levels ( $E(^2P_{1/2}^o) = 0.369$  Ry) contribute negligibly to the rate coefficients; at  $T = 20,000$  K the Maxwellian factor  $\exp(-E/kT) \approx e^{-8}$ , and decreasing accordingly for  $E > 1$  Ry in Eq. (3).

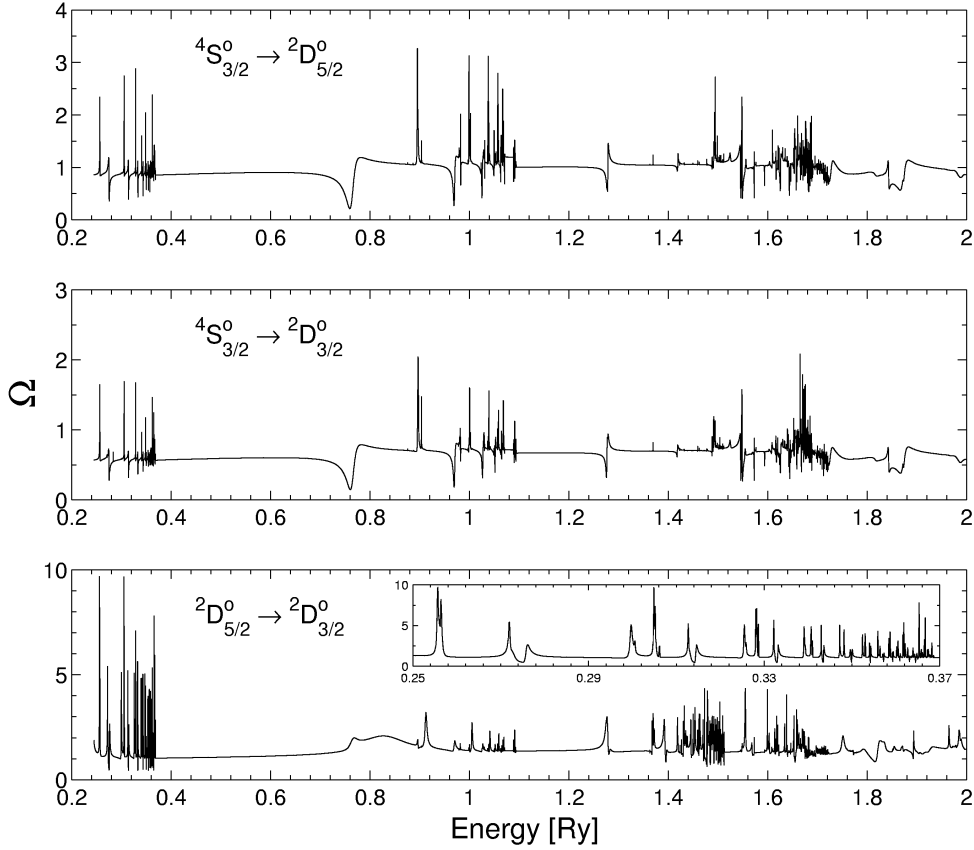
In the calculation of [O II] line ratios we employ the transition probabilities from Zeippen (1982). Eissner and Zeippen (1981) computed the  $A$ -values for [O II] transitions taking full account of the magnetic dipole M1 operator, and they showed that in the high density limit the line ratio

$$\lim_{N_e \rightarrow \infty} \frac{I(3729)}{I(3726)} = \frac{6 A(^2D_{5/2}^o - ^4S_{3/2}^o)}{4 A(^2D_{3/2}^o - ^4S_{3/2}^o)} = 0.35. \quad (5)$$

## 3 RESULTS AND DISCUSSION

Fig. 1 shows the fine structure BPRM collision strengths  $\Omega(^4S_{3/2}^o - ^2D_{5/2}^o)$ ,  $\Omega(^4S_{3/2}^o - ^2D_{3/2}^o)$  and  $\Omega(^2D_{5/2}^o - ^2D_{3/2}^o)$ . These figures appear to be the first clear presentation of the resonances in these collision strengths. P76 did not present detailed resonance structures except in the near-threshold region of  $\Omega(^2D_{5/2}^o - ^2D_{3/2}^o)$ . MB98 plotted these on an energy scale up to 5 Ry, well above the resonance region up to  $\sim 2$  Ry, but which does not exhibit the resonances in detail to enable comparison. An interesting feature clear from Fig. 1 is that the resonances do not play a large role in  $\Omega(^4S_{3/2}^o - ^2D_{5/2}^o)$  and  $\Omega(^4S_{3/2}^o - ^2D_{3/2}^o)$  and hence the rate coefficients for these transitions. Although they are significant in  $\Omega(^2D_{5/2}^o - ^2D_{3/2}^o)$ , collisional mixing via this transition is not important in the low density limit, which therefore depends only on the ratio of the transitions from the ground state  $^4S_{3/2}^o$  to the  $^2D_{5/2,3/2}^o$  levels. We find that this ratio is constant at  $6/4$  throughout the energy range under consideration, resonant or non-resonant values. Therefore we do not find any significant evidence of relativistic effects, which would manifest itself in a departure from this ratio. Remarkably the present total sum  $\sum_{J=5/2,3/2} \Omega(^4S_{3/2}^o - ^2D_J^o) = 1.42$ , compared to the  $LS$  coupling P76 value of 1.31, and an even earlier value of 1.36 obtained by Saraph, Seaton, and Shemming (1969).

Table 1 give the Maxwellian averaged collision strengths  $\Upsilon(T)$  for the 5-level [O II] model. At 10,000 K we obtain  $\Upsilon(^4S_{3/2}^o - ^2D_{3/2}^o) = 0.585$ , in good agreement with the earlier P76 value of 0.534, about 9% lower, but considerably higher than the M98 value of 0.422 (quoted in K99) which is 28% lower than the new value. More importantly our results disagree with MB98 for the ratio discussed above. It is this ratio that is responsible for the K99 line ratio  $I(3729)/I(3726)$  to



**Figure 1.** Collision strengths for the fine structure transitions associated with the [O II] line ratio 3729Å/3726Å. Note that  $\Omega(4S_{3/2}^{\circ} - 2D_{5/2}^{\circ})/\Omega(4S_{3/2}^{\circ} - 2D_{3/2}^{\circ}) = 1.5$  throughout. There is significant resonance enhancement in the collisional mixing transition  $2D_{5/2}^{\circ} - 2D_{3/2}^{\circ}$ ; the inset shows the near-threshold resonances on an expanded scale.

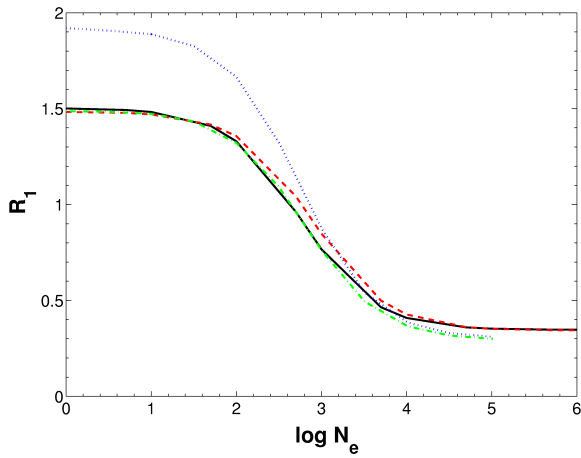
**Table 1.** Effective Maxwellian averaged collision strengths

Transition	$\Upsilon(1000\text{ K})$	$\Upsilon(5000\text{ K})$	$\Upsilon(10000\text{ K})$	$\Upsilon(15000\text{ K})$	$\Upsilon(20000\text{ K})$	$\Upsilon(25000\text{ K})$
$4S_{3/2}^{\circ} \rightarrow 2D_{5/2}^{\circ}$	0.864	0.885	0.883	0.884	0.885	0.888
$4S_{3/2}^{\circ} \rightarrow 2D_{3/2}^{\circ}$	0.590	0.587	0.585	0.585	0.585	0.588
$2D_{5/2}^{\circ} \rightarrow 2D_{3/2}^{\circ}$	1.618	1.518	1.426	1.365	1.324	1.320
$4S_{3/2}^{\circ} \rightarrow 2P_{3/2}^{\circ}$	0.299	0.307	0.313	0.318	0.322	0.327
$2D_{5/2}^{\circ} \rightarrow 2P_{3/2}^{\circ}$	0.912	0.928	0.946	0.971	1.000	1.030
$2D_{3/2}^{\circ} \rightarrow 2P_{3/2}^{\circ}$	0.571	0.589	0.605	0.624	0.644	0.664
$4S_{3/2}^{\circ} \rightarrow 2P_{1/2}^{\circ}$	0.148	0.151	0.152	0.154	0.156	0.158
$2D_{5/2}^{\circ} \rightarrow 2P_{1/2}^{\circ}$	0.383	0.392	0.402	0.414	0.428	0.441
$2D_{3/2}^{\circ} \rightarrow 2P_{1/2}^{\circ}$	0.376	0.386	0.397	0.409	0.423	0.437
$2P_{3/2}^{\circ} \rightarrow 2P_{1/2}^{\circ}$	0.277	0.284	0.291	0.300	0.310	0.321

be about 30% higher ( $\sim 2.0$ ) than the expected low-density limit of 1.5, as shown in Fig. 2.

Comparing the present relativistic BPRM results for effective collision strengths with the LS coupling results of P76 we find good agreement, mostly within a few percent, with the notable exception of  $\Upsilon(2D_{5/2}^{\circ} - 2D_{3/2}^{\circ})$ . Owing to the more extensive delineation of resonance structures in the present calculations (Fig. 1), the  $\Upsilon$  value is much higher. For example, at  $T = 10,000\text{ K}$  the P76 value is 1.168 compared to the present value of 1.426 in Table 1. On the other hand the present  $\Upsilon(2P_{3/2}^{\circ} - 2P_{1/2}^{\circ}) = 0.291$  agrees well with the P76 value 0.287 at  $T = 10,000\text{ K}$ .

Fig. 2 shows that the present collision strengths yield the line ratio  $R_1 = I(3729)/I(3726)$ , which approaches the low- and high-density limits exactly. The difference is not discernible when we use the P76 values. On the other hand the difference with MB98 is quite pronounced and approaches  $\sim 30\%$  in the low-density limit. The temperature variation between  $T = 10,000\text{ K}$  (solid line) and  $T = 20,000\text{ K}$  (dashed line) is also small, demonstrating the efficacy of this ratio as an excellent density diagnostic.



**Figure 2.** [O II] line ratio  $I(3729)/I(3726)$  vs electron density  $N_e$ : present results — solid line, Pradhan (1976) -.- dot-dashed line (nearly indistinguishable from the solid line), McLaughlin and Bell (1998) .... dotted line, at  $T = 10,000$  K. The dashed line is the line ratio at  $T = 20,000$  K.

#### 4 CONCLUSION

We have carried out new relativistic Breit-Pauli R-matrix calculations for the [O II] transitions responsible for the important density diagnostic line ratio  $3729\text{\AA}/3726\text{\AA}$ . We find no evidence of any significant departure from the earlier *LS* coupling results of Pradhan (1976). The line ratios derived from the present results also agree with the canonical limits expected on physical grounds. The new results are in considerable disagreement with the calculations of McLaughlin and Bell (1989) and the line ratios of Keenan *et al.* (1999). We also reconfirm the observational analyses of Copetti and Witzel (2002) and Wang *et al.* (2004).

#### ACKNOWLEDGMENTS

AKP would like to thank Prof. Don Osterbrock for first pointing out this problem. The computational work was carried out on the Cray X1 at the Ohio Supercomputer Center in Columbus Ohio. This work was partially supported by a grant from the U.S. National Science Foundation.

#### REFERENCES

- Aller L.H. & Hyung S., 1995, MNRAS 276, 1101  
 Aller L.H., Hyung, S. & Feibelman W. A. 1996, PASP 108, 488  
 Berrington K.A., Eissner W. & Norrington P.H., 1995, Comput. Phys. Commun. 92, 290  
 Copetti M.V.F., & Witzel B.C., 2002, A&A 382, 282  
 Creech, M.A., Seaton, M.J. & Wilson, P.M.H. 1978, Comput. Phys. Commun., 15, 23  
 Dopita M. A. & Sutherland R. S. 2003, *Astrophysics of the Diffuse Universe*, Springer-Verlag  
 Eissner, W. & Seaton, M.J. 1972, J.Phys.B, 5, 2187  
 Eissner, W. & Seaton, M.J. 1974, J.Phys.B, 7, 2533  
 Eissner, W. & Zeippen, C.J. 1981, J.Phys.B, 14, 2125

- Hummer D.G., Berrington K.A., Eissner W., Pradhan A. K., Saraph H.E. & Tully J. A., 1993, A&A 279, 298  
 Keenan F. P., Aller A. H., Bell K. L., Crawford F. L., Feibelman W. A., Hyung S., McKenna F. C. & McLaughlin B. M., 1999, MNRAS 304, 27  
 Kingsburgh R. L. & English J., 1992, MNRAS 259, 635  
 Keyes C.D., Aller L.H. & Feibelman W. A. 1990, PASP 102, 59  
 McLaughlin B. M. & Bell K.L., 1998, J. Phys. B 31, 4317  
 Montenegro M., Eissner W., Nahar S.N. & Pradhan A.K. 2005, J. Phys. B (submitted)  
 Pradhan A. K., 1976, MNRAS 177, 31  
 Wang W., Liu X.-W., Zhang Y. & Barlow M., 2004, A&A 423, 886  
 Osterbrock D.E., *Astrophysics of Gaseous Nebulae and Active Galactic Nuclei*, 1989, University Science Books, Mill Valley, California  
 Saraph, H.E., Seaton, M.J. & Shemming, J. 1969, Proc. Roy. Soc., 264, 77  
 Seaton, M.J. & Osterbrock, D.E. 1957, ApJ, 125, 66  
 The Opacity Project Team 1995, Vol. 1, Institute of Physics, London, UK  
 Zeippen, C.J. 1982, J. Phys. B, MNRAS, 198, 111